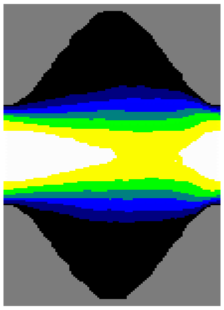

RESEARCH HIGHLIGHT
Basic Energy Sciences Program
Geosciences Subprogram

Project: Effects of Microscopic Reactions and Buoyancy on Macroscopic Transport in Geologic Media: A Lattice Gas study of Retardation and Dispersion.

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Objective: Use Lattice Gas Automata (LGA) to determine effects of surface reactions and buoyancy on macroscopic transport of solutes and colloids through geologic media; test common dispersion and retardation approximations.

Results: The Reynolds equation, widely used for modeling flow in fractures, was tested against LGA calculations for 2-D fractures with sinusoidal walls. It was shown that the Reynolds equation captures many on the effects of surface roughness on flow, but tends to overestimate fluid velocity when compared against the more exact solution afforded by LGA. The discrepancy between the two methods increased with decreasing surface separation, misalignment of the roughness, and increasing Reynolds number (figures below demonstrate flow patterns at Reynolds # 60). We believe that the discrepancies will be less for real 3-D fractures, since flow will tend to be channelized into relatively smooth-walled "tubes".

This study showed both strengths and weaknesses of LGA, the latter perhaps not appreciated by some researchers contemplating use of the technique. To minimize wall effects, we used fairly large LGA simulations, with the fracture walls separated by up to 1000 nodes. With the larger separations, it was found that very long run times were required to achieve a true steady-state flow field. Run times were effectively limited by the time required for "momentum diffusion" and equilibration between the walls and central portion of the channel. The number of LGA time steps for equilibration is $h^2/$, where h is the channel width and is the kinematic viscosity of the automaton. Since the clock time required for an LGA time step is also proportional to h, the actual clock time required for a calculation is $h^3/$. The run times were greatly reduced by "pre-conditioning" the channel with the approximate flow field expected at steady state.

Significance: This study helps define the usefulness for the Reynolds equation for modeling flow in fractures. Subtle practical limitations for the LGA technique were also discovered, and a method developed to overcome those limitations.

Publications: A paper describing this work, entitled "Applicability of the Reynolds Equation for Modeling Fluid Flow Between Rough Surfaces" has been accepted for publication by *Geophysical Research Letters*.